Coupled Simulations in Steam Methane Reformers using CFD and Reaction Kinetics

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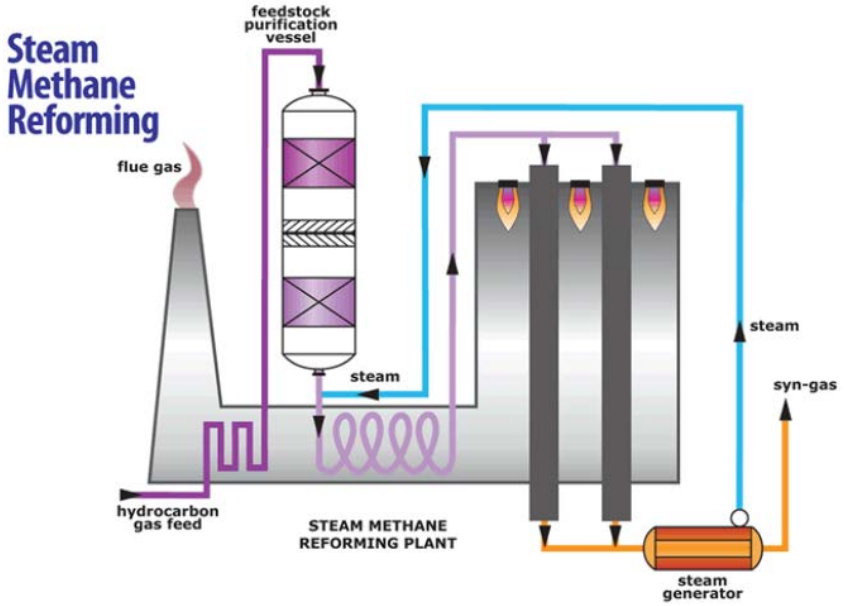
Steam Methane Reformer

- Steam Reforming: A method for producing hydrogen , carbon monoxide from hydrocarbon fuels like natural gas

- The hydrogen produced can be used for:
  - Feedstock for fuel cells
  - Hydrogenating vegetable oils for food industry
  - Industrial synthesis of ammonia (Haber process)
  - Hydrocracking of heavy petroleum fractions into lighter ones
  - Hydro-desulfurization for sulfur removal from natural gas and other refined petroleum products



http://www.eajv.ca/english/h2

High temperature (700-1100 deg C)

$CH_4 + H_2O \rightleftharpoons CO + 3\,H_2$ [Endothermic]

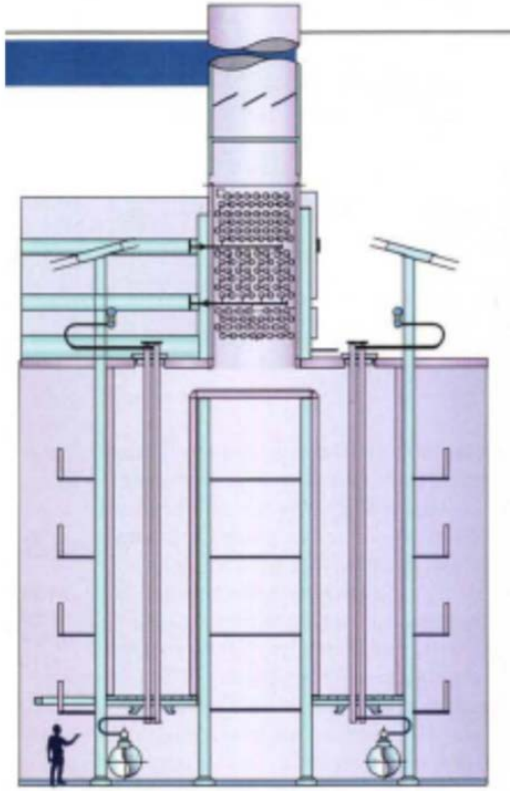
(in the presence of a metal based catalyst)

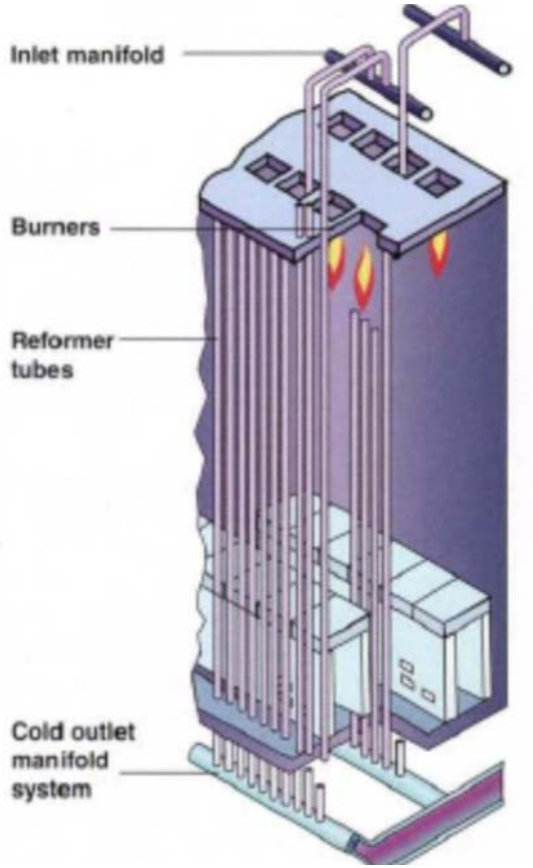
Low Temperature water gas shift reaction

$CO + H_2O \rightleftharpoons CO_2 + H_2$ [Mildly Exothermic]

Modeling Challenges

- Typical reformer furnace could have large number of burners
- Several hundred process tubes present
- Furnace dimensions are orders of magnitude larger than process tube dimensions
- Burners, process tube spacing influences flow patterns and heat flux distribution.
  - Hydrogen conversion rates affected
  - Tube wall temperatures that could lead tube failures if too high





Hydrogen production by Steam Reforming, Ray Elshout, Chemical Engineering, May 2010

Modeling Methodologies

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- **Current codes other than STAR-CCM+**
  - Highly simplified representation of firebox and 1D modeling of process side
    - Unable to capture geometry related influences
      - Recirculation zones inside the furnace – Flue gas mal distribution
      - Shadowing effects on process tubes
      - Hot spots on process tubes leading to tube failures

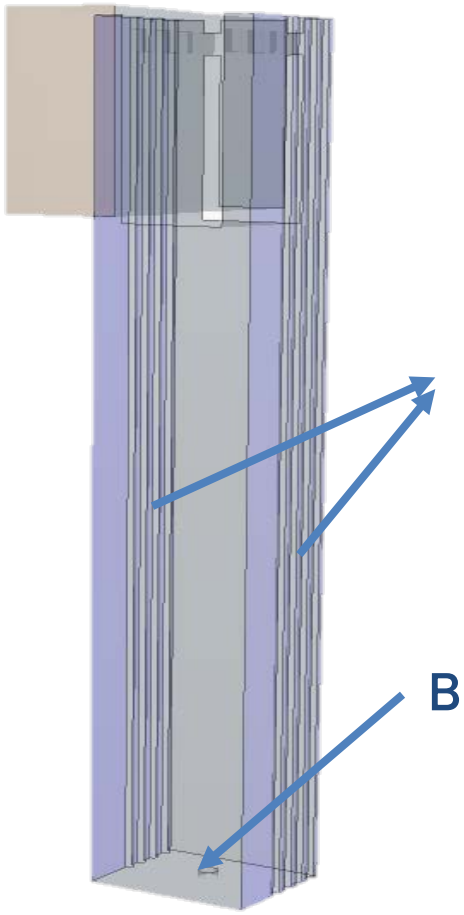
- **STAR-CCM+**
  - 3D modeling of burner side [Firebox] and 3D modeling of process side
    - Computationally expensive but possible
  - 3D modeling of Firebox and 1D modeling of process side (Reacting Channel Co-simulation)
    - Elegant way of coupling firebox side physics to tube side physics in a computationally efficient manner
    - Geometry related influences on tube wall temperatures and conversion rates effectively captured

Reacting Channel Co-Simulation in STAR-CCM+

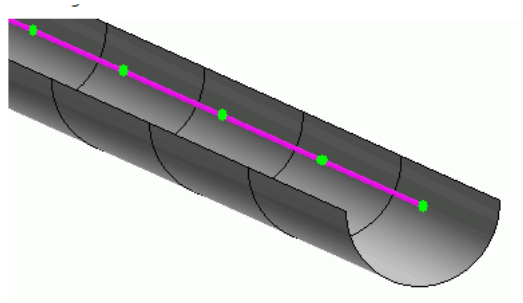
- **Gas-Phase:**
  [FireBox Side]
  - 3-D, turbulent flow
  - Combustion modeling
  - Heat transfer modeling
    - Conduction
    - Convection
    - Radiation

- **Reacting Channel:**
  [Process Side]
  - 1-D Plug Flow Reactor (PFR)
  - Process-side kinetics modeling
  - Packed bed physics for accurate heat transfer and pressure drop calculations

Model Furnace represented in 3-D



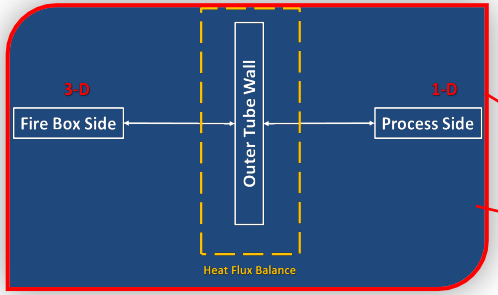
Process side physics in 1-D

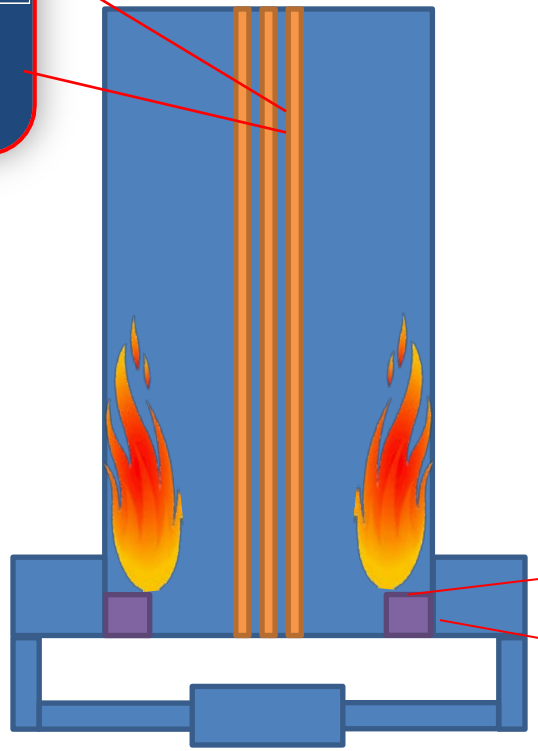


Furnace Side Modeling

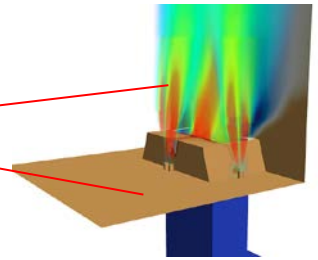
- 3-D CFD Calculations to get:
- Temperature / Heat distribution in furnace box
- Tube skin temperature
- Flame shape and length
- FGR pattern
- Radiant : Convective section heat balance
- Emissions
  - NOx
  - CO

3-D and 1-D coupling





Burner Design



Firebox Side Results

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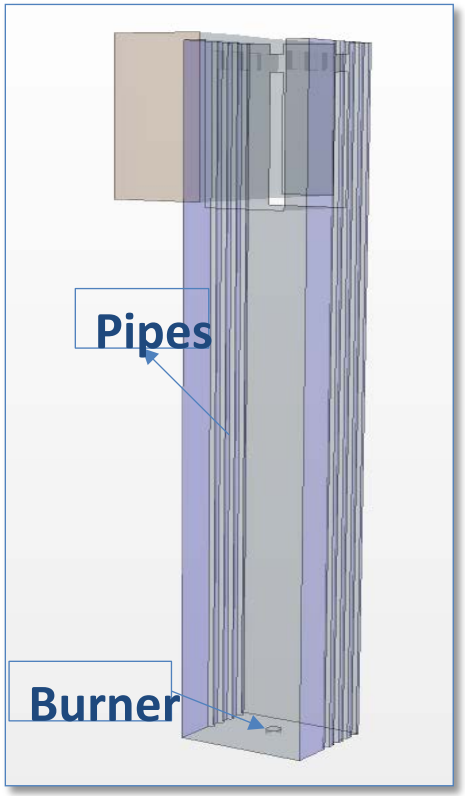
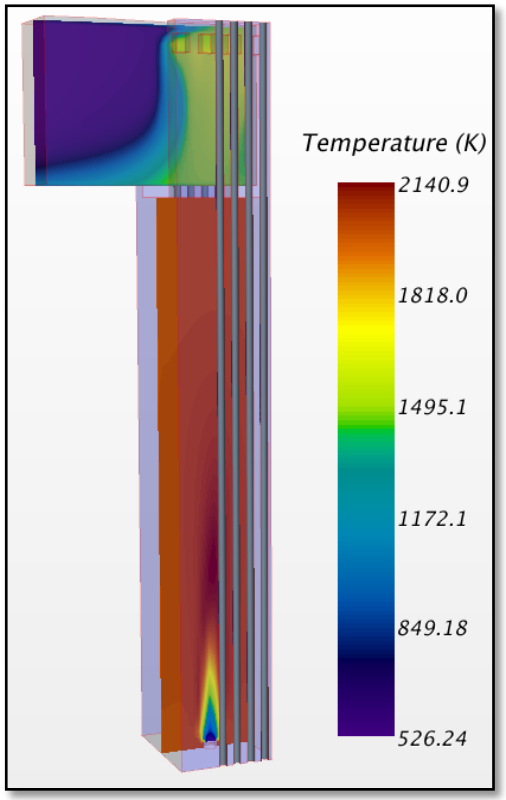
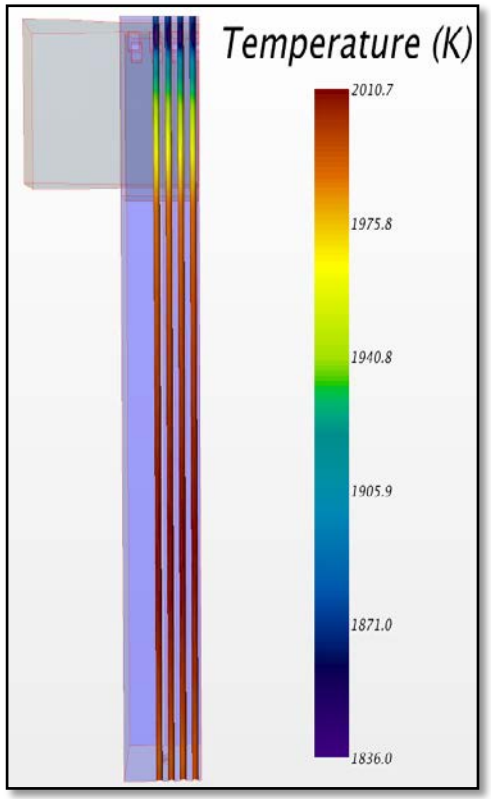
Generic Reformer



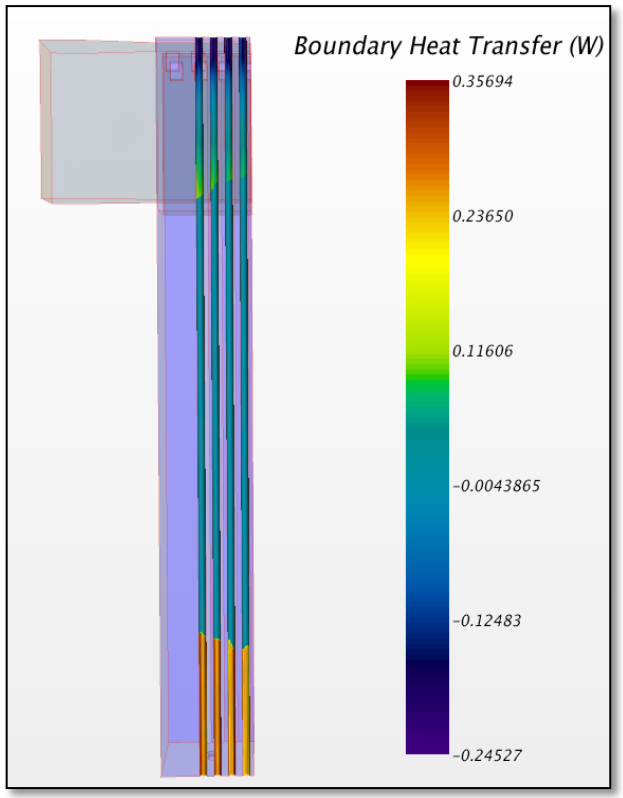
Gas Phase Temperature



Wall Temperature



Net Heat Transfer at the wall

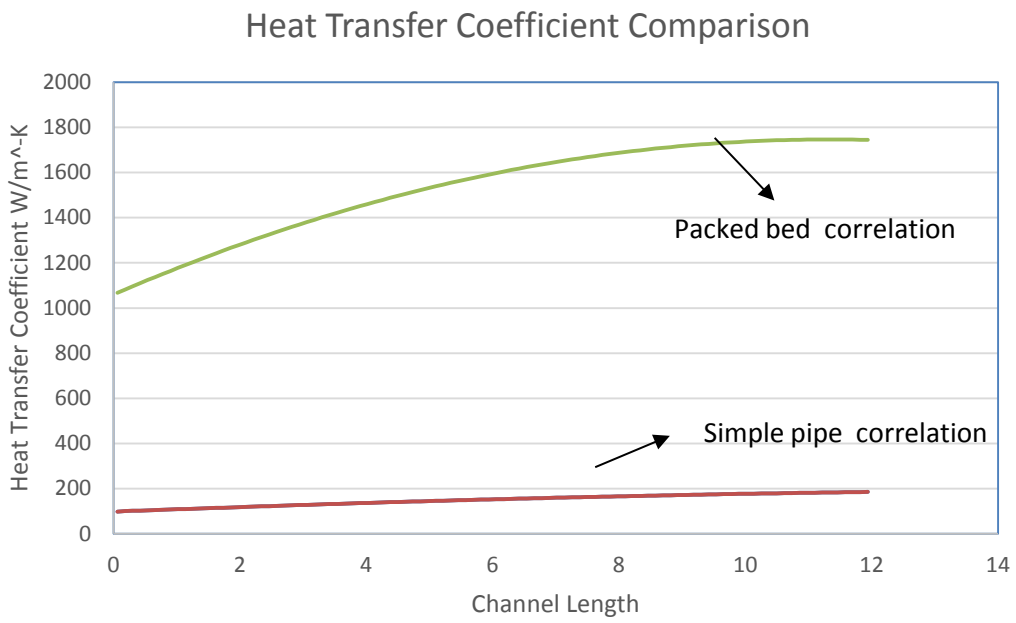


Tube Side Physics –(1)

- **Heat Transfer Coefficient Computation**
  - Simple pipe
  - Packed beds
    - Leva/Grummer
    - Beek
    - DeWasch/Froment
  - User-defined tabular input

- **Heat transfer through a packed bed has a significant effect on the performance of the equipment**

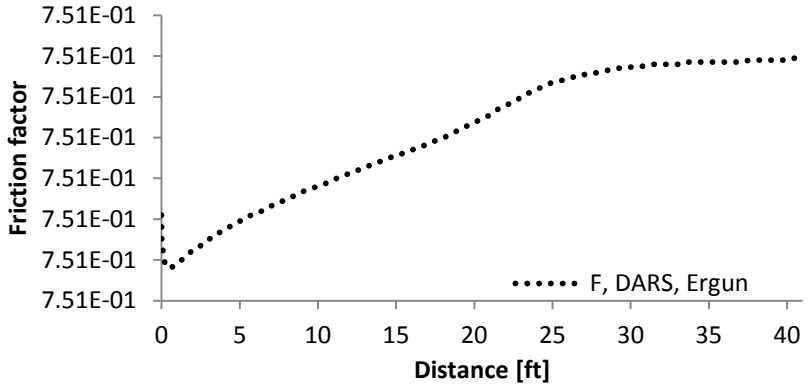
- **Much higher heat transfer coefficient values seen in packed beds than simple pipes. This significantly influences conversion rates**



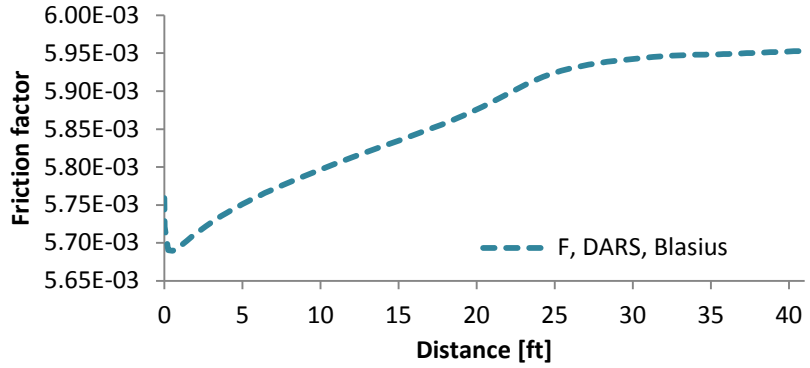
Tube Side Physics –(2)

- Pipe friction correlations for packed beds and simple pipes available
- Accurate pressure drop through packed tubes can be captured

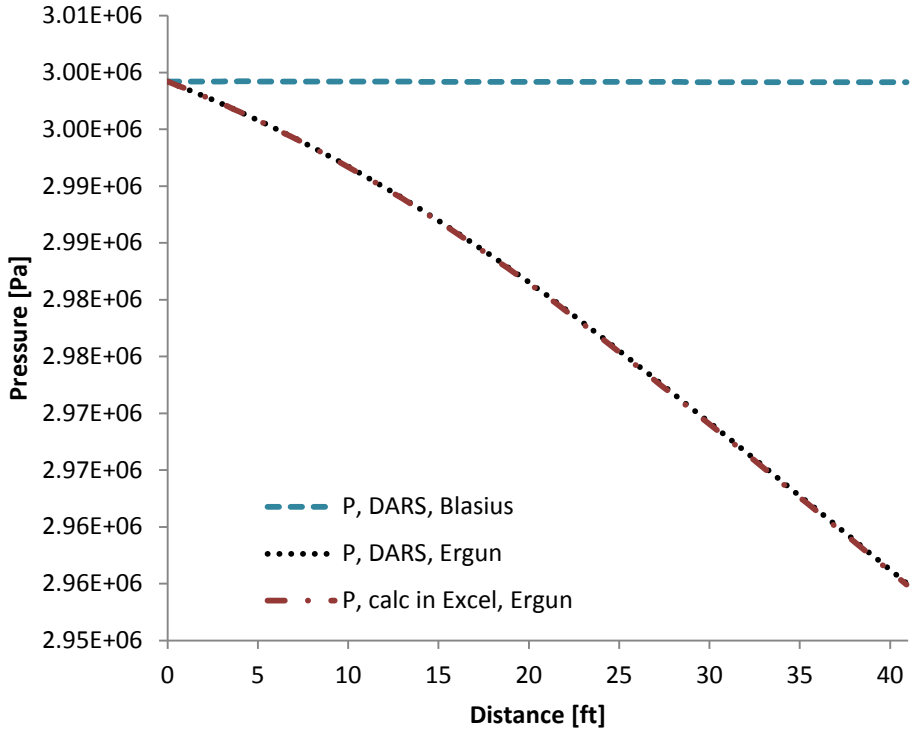
Friction factor for packed bed



Friction factor for simple pipe

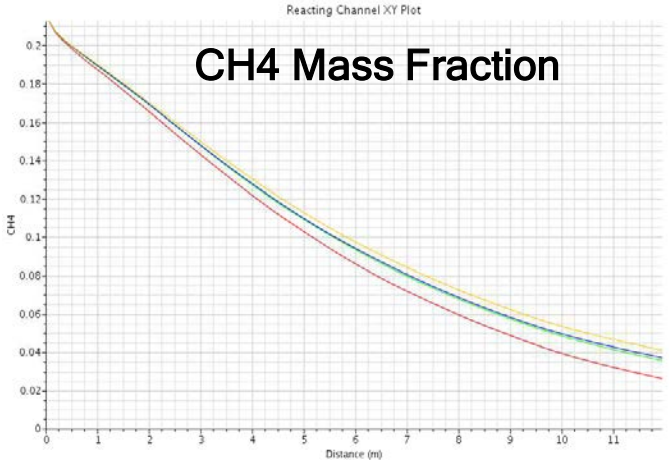


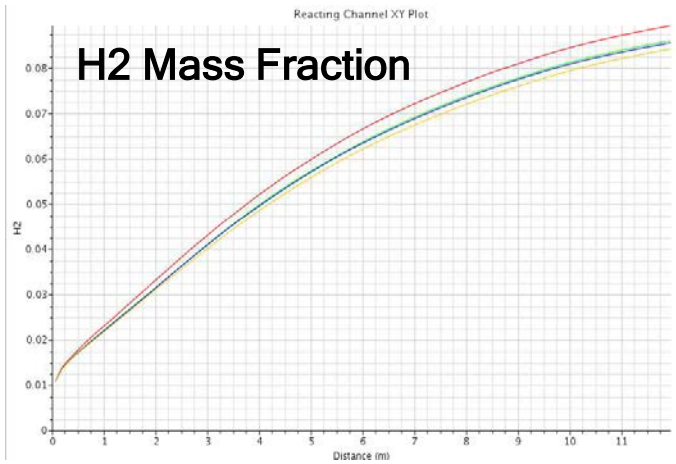
Pressure drop comparison between simple pipe and packed bed

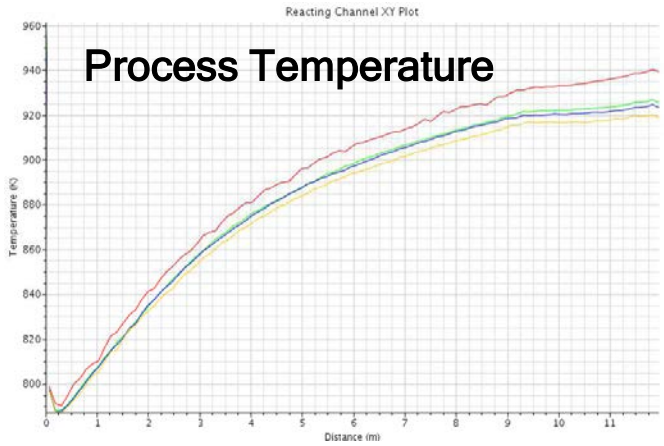


Tube Side Physics –(3)

- **Steam-Methane reforming kinetics**
  - Detailed chemistry
  - Reduced chemistry
  - User-defined kinetic rates
- **Output Quantities**
  - Methane conversion
  - Hydrogen yield
  - Process fluid temperature
  - Tube wall temperature

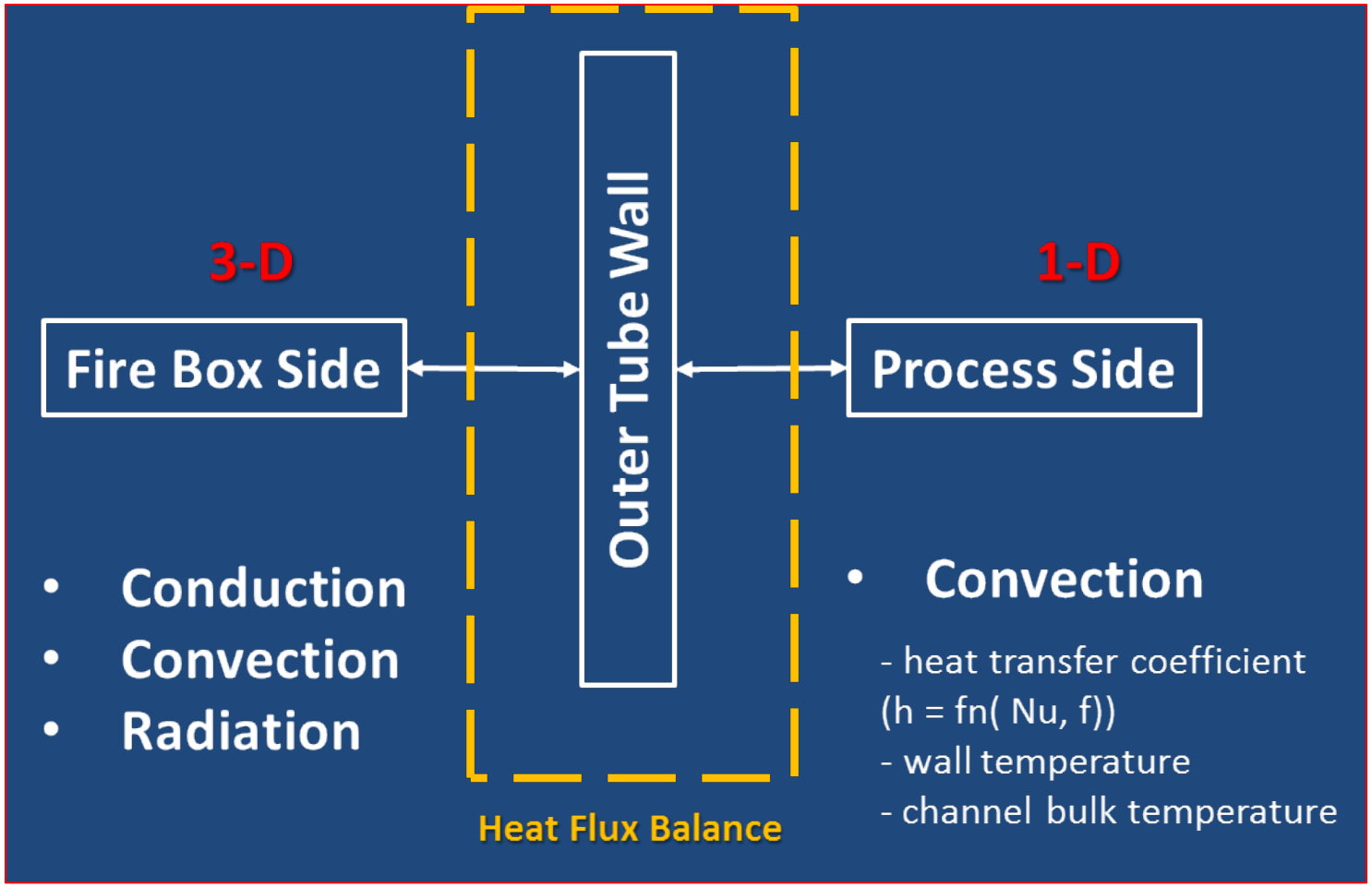






Coupling between Firebox and Process Side

Coupling achieved through energy balance at the outer tube walls



Summary

- An adequate representation of the physics on the firebox side is possible using STAR-CCM+
- Correlations for heat transfer coefficient and pressure drop enables simulations of catalytic processes like SMR to be effectively simulated using reacting channel co-simulation
- Flexible kinetics description for process side enables users to optimize process side chemistry for accurate description of reactant conversion and product yields